

CLAIMS

What is claimed is:

1. A method for comparing a query peptide to a plurality of database peptides comprising the steps of:
- (a) constructing an index table, said index table comprising a plurality of records corresponding to a plurality of allowed mass values, said records comprising zero or more fields, said constructing step comprising the steps of:
 - (i) selecting a first peptide from said plurality of database peptides;
 - (ii) calculating a plurality of associated masses for said first peptide;
 - (iii) selecting a first associated mass from said plurality of associated masses;
 - (iv) referencing a first record from said plurality of records, said first record corresponding to said first associated mass;
 - (v) entering a first field into said first record, said first field comprising a first peptide index referencing said first peptide;
 - (vi) repeating steps (iii)-(v) for at least one other associated mass from said plurality of associated masses;
 - (vii) repeating steps (i)-(vi) for at least one other peptide from said plurality of database peptides; and
 - (b) generating a plurality of comparison scores, said plurality of comparison scores corresponding to said plurality of database peptides, said generating step comprising the steps of:
 - (i) generating a plurality of query mass values for said query peptide;
 - (ii) selecting a first query mass value from said plurality of query mass values;
 - (iii) referencing a second record from said plurality of records, said second record corresponding to said first query mass value;

- 27 (iv) selecting a second field from said second record, said second field
 28 comprising a second peptide index;
 29 (v) selecting a first comparison score from said plurality of comparison
 30 scores, said first comparison score corresponding to said second
 31 peptide index;
 32 (vi) incrementing said first comparison score;
 33 (vii) repeating steps (ii)-(vi) for at least one other query mass value
 34 selected from said plurality of query mass values.

1 2. The method of claim 1 wherein said generating step (b)(i) comprises the step of
 2 performing mass spectroscopy on said query peptide.

1 3. The method of claim 2 wherein said mass spectroscopy is performed by a method
 2 selected from the set consisting of: Fourier transform ion cyclotron resonance
 3 ("FTICR"), quadrupole mass spectroscopy, ion trap mass spectroscopy, and time-
 4 of-flight mass spectroscopy.

1 4. The method of claim 1 wherein said calculating step (a)(ii) comprises the step of
 2 calculating a plurality of associated masses for said first peptide, said plurality of
 3 associate masses comprising a plurality of primary masses and a plurality of
 4 complementary masses.

1 5. The method of claim 1 wherein said generating step (b) further comprises the step
 2 of multiplying said first comparison score by a weight value, wherein said weight
 3 value is a function of the type of mass value.

1 6. The method of claim 5 wherein said type of mass value is selected from the group
 2 consisting of: y-ion, b-ion, peak mass, and complementary mass.

1 7. A method for comparing a query peptide to a plurality of database peptides
 2 comprising the steps of:

- 3 (a) constructing a first index table, said first index table comprising a first
- 4 plurality of records corresponding to a plurality of allowed mass values,
- 5 said records comprising zero or more fields; and
- 6 (b) constructing a second index table, said second index table comprising a
- 7 second plurality of records corresponding to said plurality of allowed mass
- 8 values, said records comprising zero or more fields; and
- 9 (c) calculating a plurality weight values, said weight values set according to
- 10 the predictive value of said first and second index tables.

1 8. A method for comparing a modified query peptide to a plurality of database
2 peptides comprising the steps of:

- 3 (a) generating a plurality of query mass values for said query peptide;
- 4 (b) identifying a set of query mass values from said plurality of query mass
- 5 values, wherein said set corresponds to modified mass values;
- 6 (c) determining a spectral range for said query peptide;
- 7 (d) subdividing said spectral range into a plurality of equal intervals;
- 8 (e) performing a plurality of searches on said plurality of equal intervals.

1 9. The method of claim 8 further comprising the step of excluding said set of query
2 mass values.

1 10. The method of claim 8 further comprising the step of adjusting said set of query
2 mass values.

1 11. A method for comparing a query peptide to a plurality of database peptides
2 comprising the step of constructing an index table, said index table comprising a
3 plurality of records corresponding to a plurality of allowed mass values, said
4 records comprising zero or more fields, said constructing step comprising the
5 steps of:

- 6 (i) selecting a first peptide from said plurality of database peptides;
- 7 (ii) identifying a modification site on said first peptide;

- 8 (iii) applying a modification to said modification site, producing a first
- 9 modified peptide;
- 10 (iv) calculating a plurality of associated masses for said first modified peptide;
- 11 (v) selecting a first associated mass from said plurality of associated masses;
- 12 (vi) referencing a first record from said plurality of records, said first record
- 13 corresponding to said first associated mass;
- 14 (vii) entering a first field into said first record, said first field comprising a first
- 15 peptide index referencing said first peptide;
- 16 (viii) repeating steps (v)-(vii) for at least one other associated mass from said
- 17 plurality of associated masses;
- 18 (ix) repeating steps (i)-(viii) for at least one other peptide from said plurality of
- 19 database peptides.

1 12. The method of claim 11 wherein said identification step (ii) comprises the step of
 2 identifying a modification site selected from the group consisting of: a
 3 phosphorylation site, an oxidation site, and a substitution site.

1 13. The method of claim 12 wherein said phosphorylation site comprises an amino
 2 acid selected from the group consisting of: serine, threonine, and tyrosine.

1 14. The method of claim 12 wherein said oxidation site comprises an amino acid
 2 selected from the group consisting of: cysteine and methionine.

1 15. The method of claim 12 wherein said substitution site comprises an amino acid
 2 selected from the group consisting of: glutamine, glutamate, asparagine, and
 3 aspartate.